Using SpF to Achieve Petascale for Legacy Pseudospectral Applications

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Background/Motivation

NASA HEC supports at least 5 pseudospectral applications:

Spherical Geometry

- DYNAMO
- MoSST
- ASH

Cartesian Geometry

- HPS
- DDSCAT

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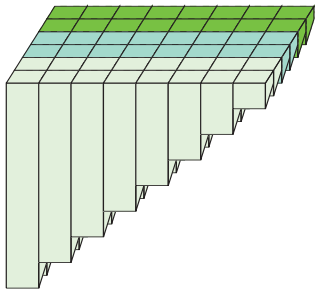
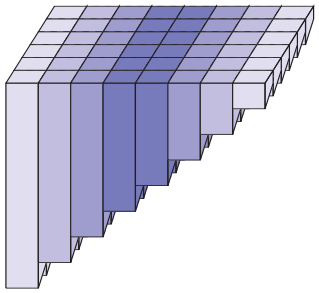
- constrains **grid resolution**

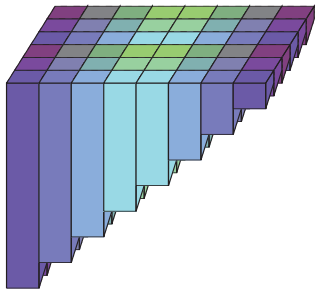
(Mostly) my fault!

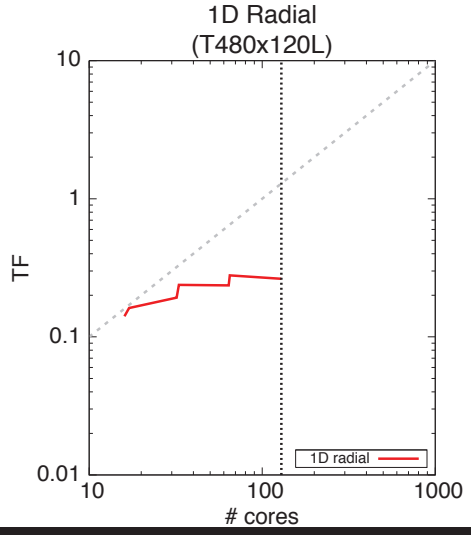
Consequences of 1D decomposition

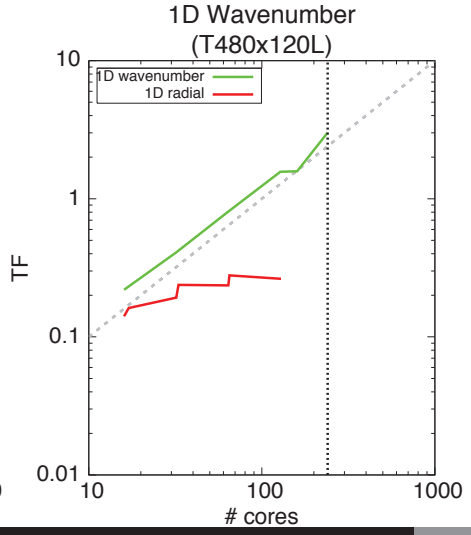
Scaling Legendre Transforms

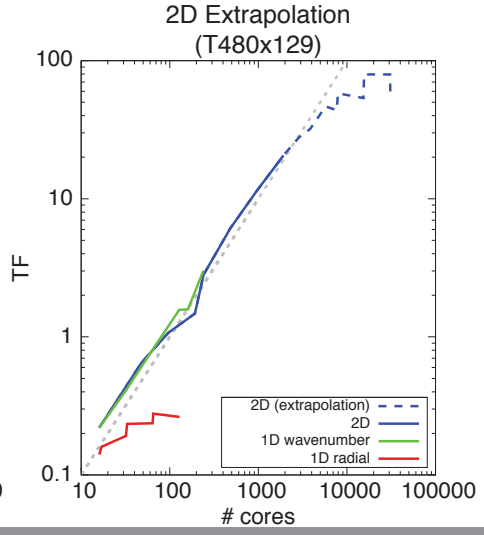












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Pseudospectral methods have an elegant structure that provides quite interesting challenges from a software design perspective

- Alternate between *local* computation and all-to-all communication
- Complicated data structures (harmonic truncation)
- Nontrivial load-balance
- Most numerical calculations can be done with vendor-optimized libraries

Solution - SpF

SpF (Spectral Framework) is a software framework tailor designed to maximize the performance and scalability of pseudospectral applications.

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Specific design goals: (separation of concerns)

- **Support multiple geometries (sphere, box, ...?)**
- Manage: domain decomposition, transpose, and I/O operations
- Leverage optimized numerical libraries
- Support async communication, hybrid-parallelism and HW accelerators
- Enable *decomposition independent* formulation of applications
- Allow user extensions/refinements (OO)
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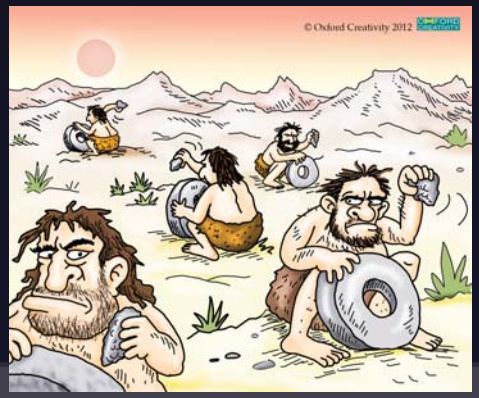
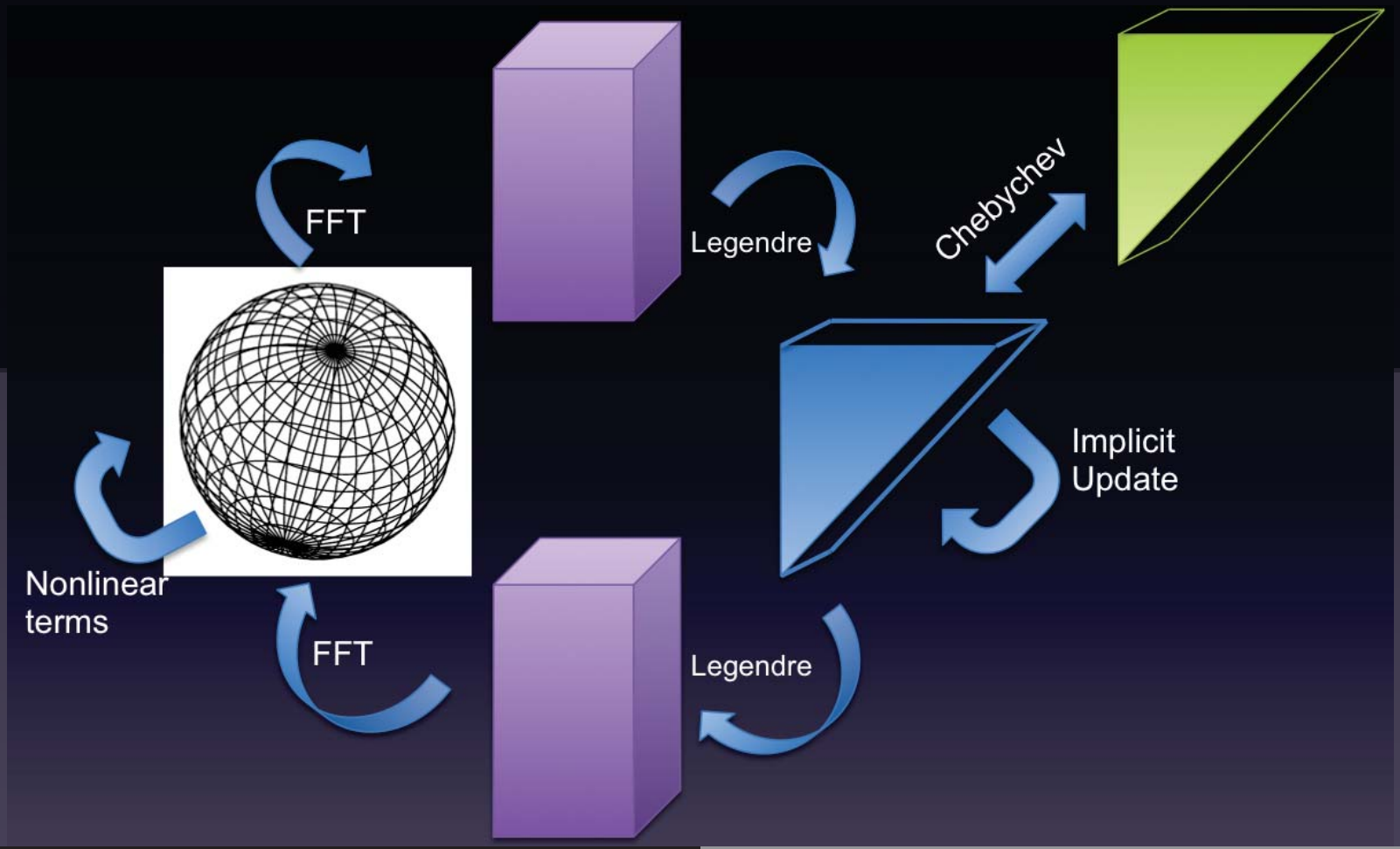
Benefits of adopting SpF



- Less duplication of effort
  - Parallel “transforms” — Legendre, LU Decomposition, etc.
  - Tedious/fragile transpose implementations
- Reduced effort to exploit new architectures/accelerators
- Readily adopt/share performance innovations within the community

Challenges and Complications



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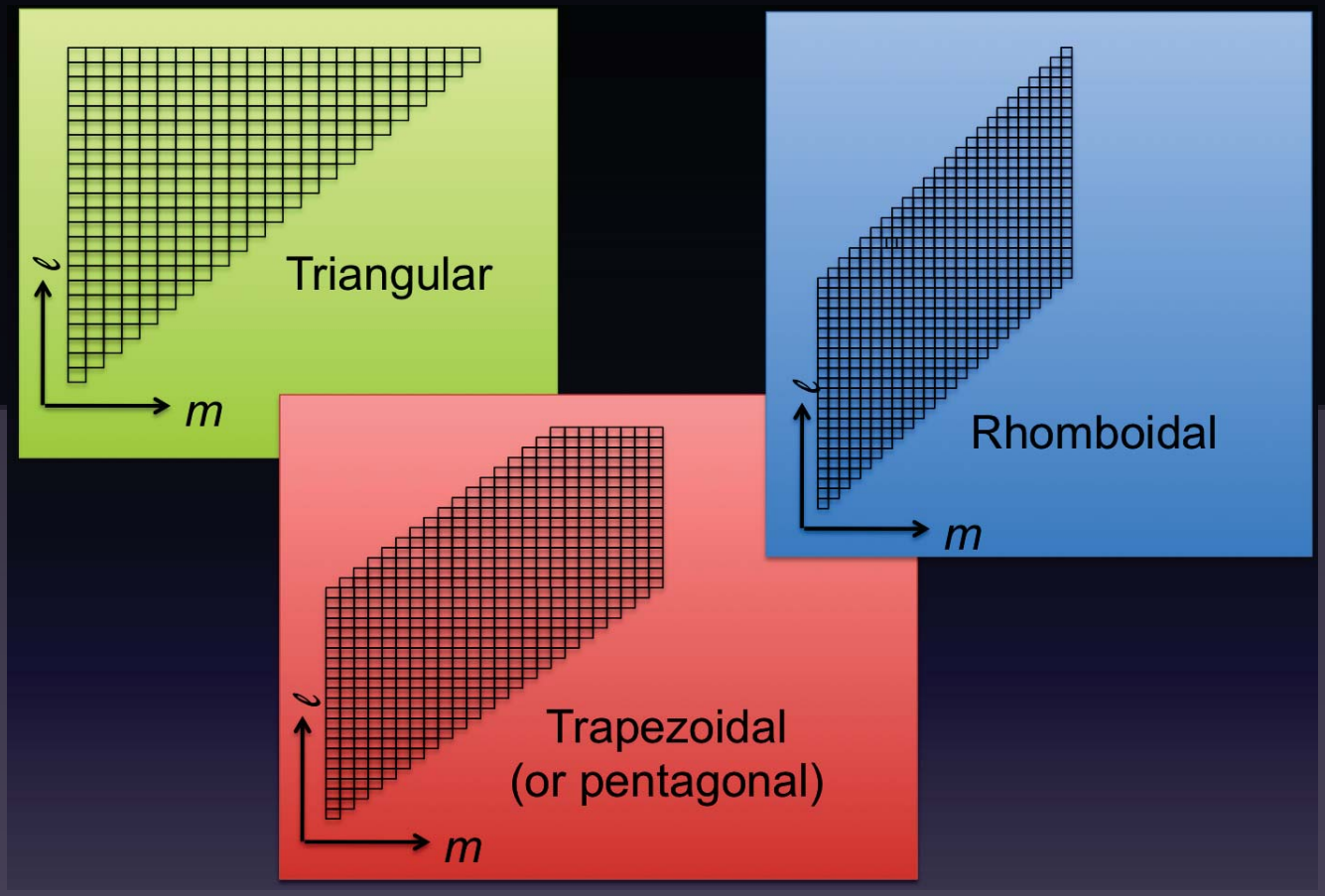

SpF: The Secret Sauce

Each transform can be expressed as a union of independent, atomic (indivisible) numerical 'kernels' $\{K_1, K_2, \ldots, K_n\}$.

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These provide a natural partition of the computational domain:

$$(X, d_x) = \left((\tilde{X}_q^1, d_x^1 \otimes q^1\right) \oplus \left(\tilde{X}_q^2, d_x^2 \otimes q^2\right) \oplus \ldots \oplus \left(\tilde{X}_q^n, d_x^n \otimes q^n\right)$$

$$(Y, d_y) = \left(\tilde{Y}_q^1, d_y^1 \otimes q^1\right) \oplus \left(\tilde{Y}_q^2, d_y^2 \otimes q^2\right) \oplus \ldots \oplus \left(\tilde{Y}_q^n, d_y^n \otimes q^n\right)$$

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Legendre

$$d_x^m = \{\ell\}_{\ell=m}^{\ell^{\max}} \otimes \{m\}$$
$$d_y^m = \{\theta_i\}_{i=1}^{n_i} \otimes \{m\}$$
$$q = q^m = \{r_k\}_{k=1}^{k=n_k} \otimes \{v_r, v_\theta, \ldots\}$$

FFT

$$d_x = \{m\}_{m=0}^{m^{\max}}$$
$$d_y = \{\phi_j\}_{j=1}^{n_j}$$
$$q = \{\theta_i\}_{i=1}^{i=n_i} \otimes \{r_k\}_{k=1}^{n_k} \otimes \{v_r, v_\theta, \ldots\}$$

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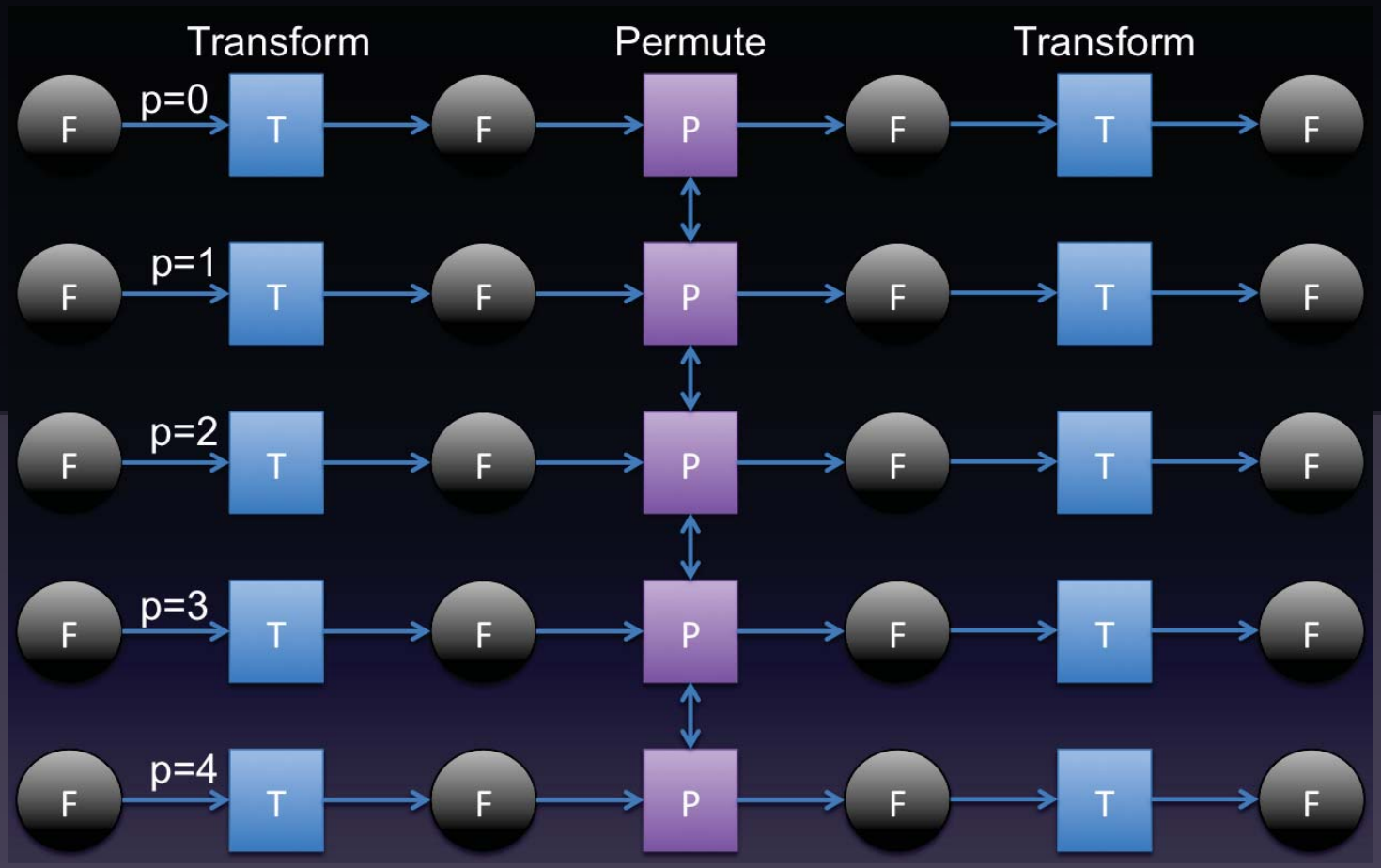
- Integrator - time integration (CN, AB, ...)

SpF: Implementation details

- Object-oriented design (ala Fortran 2003)
  - Applications built by *extending* SpF abstractions
  - User-extensions that can be shared by community
- Aggressive use of test-driven development (TDD) & pFUnit
  - More that 300 unit tests
  - Runs on at least 3 compilers (Intel, GNU, NAG)
- Demonstrated with multi-layer shallow water
- Not quite ready for distribution
  - Open source release planned (tedious paperwork)
  - Project-level release could be expedited

How SpF sees an application



IndexSpace - Cartesian Example

```
1  use SpF_mod
2  class (IndexSpace) :: cartesian
3  type (RangeAxis) :: xAxis, yAxis, zAxis
4
5  xAxis = RangeAxis('x', nx)
6  yAxis = RangeAxis('y', ny)
7  zAxis = RangeAxis('z', nz)
8
9  allocate(cartesian, source= xAxis*yAxis*zAxis)
```

IndexSpace - Cartesian Bundle

```
 1  use Spf_mod
 2  class (IndexSpace) :: cartesianBundle
 3  type (RangeAxis) :: xAxis, yAxis, zAxis
 4  type (StringAxis) :: qtys
 5
 6  xAxis = RangeAxis('x', nx)
 7  yAxis = RangeAxis('y', ny)
 8  zAxis = RangeAxis('z', nz)
 9  qtys = StringAxis('qty', ['W', 'Z', 'S', 'P'])
10
11  allocate(cartesianBundle, source= &
12     &    xAxis*yAxis*zAxis*qtys)
```

IndexSpace - Triangular Truncation

```
1  use SpF_mod
2  class (IndexSpace) :: tDomain
3  class (OuterProductSpace) :: modeAxis
4  type (RangeAxis) :: rAxis
5
6  modeAxis = RangeAxis('m', 0, 0) * RangeAxis('ell', 0, Lmax)
7  Allocate(tDomain, source=mode)
8
9  do m = 1, mMax
10     modeAxis = RangeAxis('m', m, m) * RangeAxis('ell', m, Lmax)
11     allocate(tDomain, source= tDomain + modeAxis)
12 end do
13
14 allocate(tDomain, source= RangeAxis('r',nn)*tDomain)
```

Automating the transpose

First we translate the index space into a labelled table:

ℓ	m	r	f
0	0	1	'S'
1	0	1	'S'
⋮			
10	7	10	'Z'
⋮			

ℓ	m	r	f
7	2	3	'W'
7	2	4	'W'
⋮			
0	12	2	'P'
⋮			

Automating the transpose

Then we append process and offset metadata:

ℓ	m	r	f	PE	δ
0	0	1	'S'	0	0
1	0	1	'S'	0	1
⋮				⋮	
10	7	10	'Z'	8	15
⋮				⋮	

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7	2	3	'W'	0	0
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⋮				⋮	
0	12	2	'P'	8	15
⋮				⋮	

Then we "co-sort" the tables to find source/destination for each element

ℓ	m	r	f	p_{src}	δ_{src}	p_{dest}	δ_{dest}
0	0	1	'S'	0	0	3	7
1	0	1	'S'	0	1	10	1
⋮				⋮		⋮	
10	7	10	'Z'	8	15	2	9
⋮				⋮		⋮	

Automating the transpose

For a 2-phase (nested) tranpsopse, we append the rank for each phase

ℓ	m	r	f	PE_0	PE_1	δ
0	0	1	'S'	0	0	0
1	0	1	'S'	0	0	1
⋮				⋮		
10	7	10	'Z'	8	2	15
⋮				⋮		

ℓ	m	r	f	PE_0	PE_1	δ
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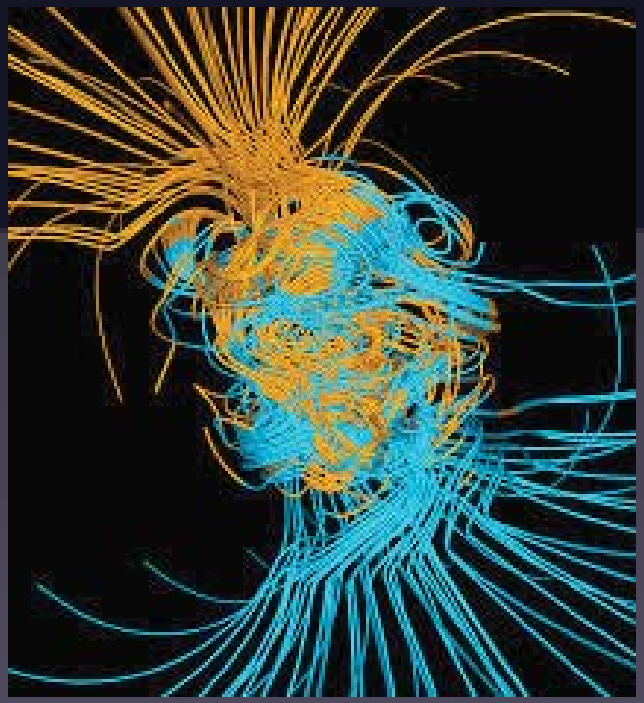
DYNAMO

Author: Gary Glatzmaier

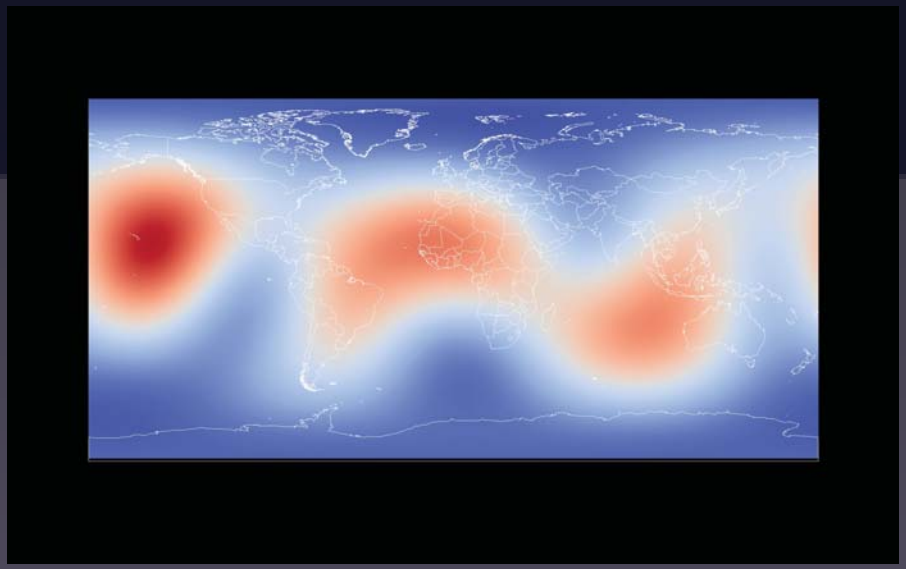


Primary configuration

- Azimuthal wavenumbers distributed over PEs
- Constraint $N_p <= N_m$
- Supports variant spectral truncations and variant hyperviscosity terms

MoSST

Author: Weijia Kuang



Primary configuration

- One dimensional Distribution over PEs at all stages
- Constraint: $N_p \leq N_m$
- Constraint: $N_p \leq N_r$
- Constraint: All Spherical transforms (Legendre and FFT) are in the same process

Adopting SpF - general strategy

1. **Establish regression tests and data for baseline.**
   - Invest in achieving *strong reproducibility*
   - Turn off optimization and turn on debugging flags
2. Proceed with incremental changes that preserve results
3. Commit to repository after each success.
4. Minor roundoff issues may be encountered
   - Isolate cause, then update baseline regression data
   - Bracket change in repository

Adopting SpF - copy to/from legacy data structures

1. Declare a FieldList object
2. Create a procedure that copies an array into a Field
3. For each contiguous array
   1. Define corresponding IndexSpace domain object
   2. Call append() method on FieldList
   3. insert call to copy procedure just prior to use

Adopting SpF - Kernel Factory

1. Create a new module:
   1. Define a derived type that *extends* KernelFactory
   2. Implement methods that compute Kernel IndexSpace (I/O)
   3. Define a derived type that *extends* Kernel
   4. Implement apply() method that wraps actual computation
2. Declare and initialize in main code:
   1. new Factory defined above
   2. Distributor, Permutor
   3. TaskList, and 2 FieldLists (in and out)
   4. Build task list, and field lists using distributor and factory
   5. Build permutor object connecting previous transform to new
3. Use in main loop:
   1. Insert call to apply() method of TaskList object

Adoption status

MoSST

- Now uses SpF permutations

DYNAMO

- SpF conversion completed for
  - Legendre transforms
  - Quadratic convolution
  - Stream to vector (i.e. $\{W, Z, \ldots\} \longrightarrow \{v_r, v_\theta, \ldots\}$)
  - Permutations (including to/from legacy layout)
- Took $\approx$ 1 week for expert (me)
  - Lots of ugly shortcuts
- Issues encountered with implicit update step
  - Could “cheat”
  - Will use experience to instead improve framework

Example - top declaration

```
1  type (SimpleMpiDistributor) :: d
2  type (FieldList) :: leg_in, leg_out, NL_in, NL_out
3  type (LegendreFactory) :: legFactory
4  type (NL_ConvolutionFactory) :: NL_Factory
5  type (PartitionedAlgorithm) :: legTasks, NL_tasks
6  type (SimpleMpIPermutor) :: perm
7  class (IndexSpace) :: initialDomain
8
9  d = SimpleMpiDistributor(MPI_communicator)
10 legFactory = LegendreFactory(mMax=1023)
11 NL_Factory = NL_ConvolutionFactory(ni, nk)
12 initialDomain = ...
```

Example - initialization

```
1  legTasks = d%distribute(legFactory, initialDomain)
2  leg_in = FieldList(legTasks,'in')
3  leg_out = FieldList(legTasks,'out')
4
5  NL_tasks = d%distribute(NL_Factory, leg_in)
6  NL_in = FieldList(NL_tasks,'in')
7  NL_out = FieldList(NL_tasks,'out')
8
9  perm = SimpleMpiPermutor(MPI_communicator, leg_out, NL_in)
```

Example - execute

```
1  ...
2  call legTasks%apply(leg_in, leg_out)
3  call perm%permute(leg_out, NL_in)
4  call NL_tasks%apply(NL_in, NL_out)
5  ...
```

Variations

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1 ! Alternate load balancing strategy
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3  type (RoundRobinDistributor) :: d

5  ! Alternative permutation strategy
6  ! type (SimpleMpiPermutor) :: perm
7  type (SomeOtherPermutor) :: perm

9  ! Alternative Legendre implementation
10 ! type (LegendreFactory) :: legFactory
11 type (AltLegFactory) :: legFactory
```

Next steps

- Finish ports of DYNAMO, MoSST, HPS, DDSCAT
- Improve framework
  - Generalize/optimize Permutor classes
    - Allow for multiple sources
    - Allow for “subsetting”
    - Implement multiphase transpose (ala Nick Featherstone)
  - Extend/improve kernels
    - Better mechanism for defining offsets
    - Allow for multiple sources/destinations
    - Allow for “fat” kernels that do internal communication (e.g. implicit treatment of coriolis)
- Release SpF as open source

Credits

- NASA High End Computing program for supporting this work
- Gary Glatmaier - for providing DYNAMO as an interesting challenge

Questions?